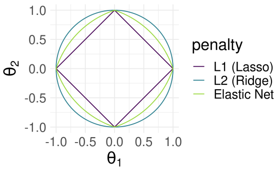
Introduction to Machine Learning

Regularization
Elastic Net and regularized GLMs

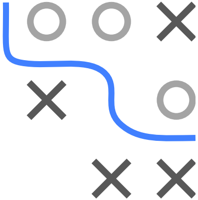


Learning goals

- Compromise between L1 and L2
- Regularized logistic regression

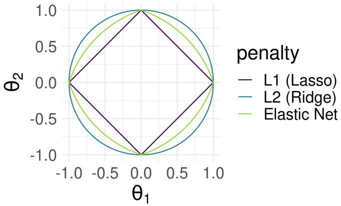
ELASTIC NET AS L1/L2 COMBO

▸ Zou and Hastie 2005



$$\mathcal{R}_{\text{elnet}}(\boldsymbol{\theta}) = \sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 + \lambda_1 \|\boldsymbol{\theta}\|_1 + \lambda_2 \|\boldsymbol{\theta}\|_2^2$$

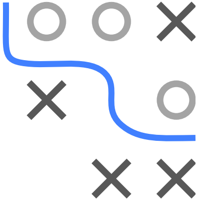
$$= \sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 + \lambda \left((1-\alpha) \|\boldsymbol{\theta}\|_1 + \alpha \|\boldsymbol{\theta}\|_2^2 \right), \ \alpha = \frac{\lambda_2}{\lambda_1 + \lambda_2}, \lambda = \lambda_1 + \lambda_2$$



- 2nd formula is simply more convenient to interprete hyperpars; λ controls how much we penalize, α sets the "L2-portion"
- Correlated features tend to be either selected or zeroed out together
- Selection of more than n features possible for $p > n$

SIMULATED EXAMPLE

50 data sets with $n = 100$ for setups: $y = \mathbf{x}^T\boldsymbol{\theta} + \epsilon; \quad \epsilon \sim N(0,1); \quad \mathbf{x} \sim N(0, \Sigma)$:



Ridge better for corr. features:

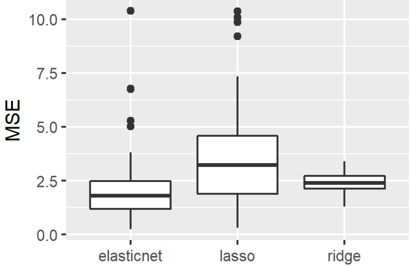
$$\boldsymbol{\theta} = (\underbrace{2,\ldots,2}_{5}, \underbrace{0,\ldots,0}_{5})$$

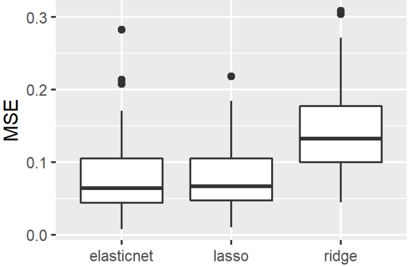
$$\Sigma_{k,l} = 0.8^{|k-l|}$$

Lasso better for sparse without corr.:

$$\boldsymbol{\theta} = (2,2,2,\underbrace{0,\ldots,0}_{7})$$

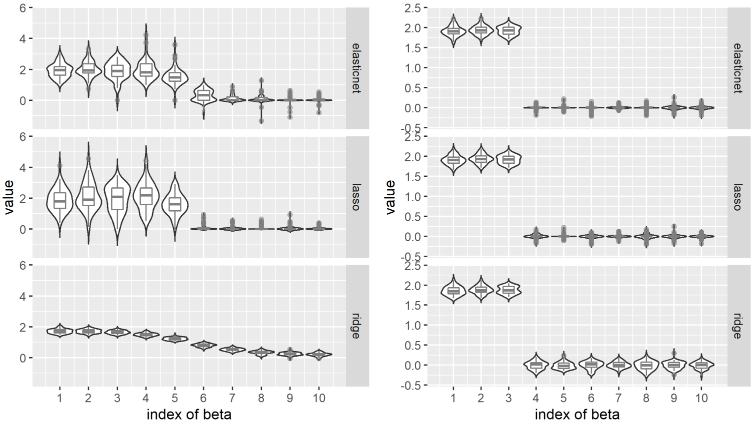
$$\Sigma = I_p$$

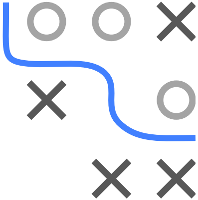




$\Longrightarrow$ elastic net handles both cases well

SIMULATED EXAMPLE / 2

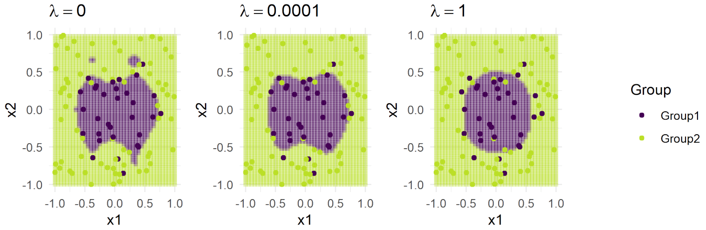




LHS: ridge cannot perform variable selection compared to lasso/e-net.
Lasso more frequently ignores relevant features than e-net (longer tails in violin plot).
RHS: ridge estimates of noise features hover around 0 while lasso/e-net produce 0s.

REGULARIZED LOGISTIC REGRESSION

- Penalties can be added very flexibly to any model based on ERM
- E.g.: $L1$- or $L2$-penalized logistic regression for high-dim. spaces and feature selection
- Now: LR with polynomial features for x_1, x_2 up to degree 7 and L2 penalty on 2D “circle data” below



- $\lambda = 0$: LR without penalty seems to overfit
- $\lambda = 0.0001$: We get better
- $\lambda = 1$: Fit looks pretty good